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Louis J. Allamandola

NASA Ames Research Center, Mail Stop 245-6, Moffett Field, CA 94036-1000

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ASTRONOMICAL INFRARED SPECTROSCOPY: FUTURE OBSERVATIONAL DIRECTIONS

Edited by Sun Kwok



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Louis J. Allamandola
NASA Ames Research Center, Mail Stop 245-6,
Moffett Field, CA 94036-1000

ABSTRACT ISO, the Infrared Space Observatory, is capable of measuring spectra across most of the mid-infrared. Nearly 19% of this spectral band has never been studied due to telluric obscuration, and 21% only partially investigated with airborne platforms. Thus ISO has the potential to nearly double our knowledge of the mid-IR spectroscopic properties of the cosmos, revolutionizing our understanding of its chemical make-up. Absorption spectroscopy of dense molecular clouds will shed light on the D/H ratio in interstellar ices, the importance of CO_2 , O_3 , and nitriles in these ices, and the chemistry of these ices. Absorption spectroscopy of dust in the diffuse interstellar medium will reveal the nature and abundance of the organics and silicates present as well as their variation across the galaxy, and may establish the D/H ratio in the diffuse medium. ISO is particularly well suited to pioneer the diffuse medium due to the low level background radiation and the high instrumental sensitivity. Emission spectroscopy of PAHs and related compounds in (proto-) planetary nebulae, reflection nebulae, HII regions, and galactic nuclei will probe the D/H ratio in these carbonaceous materials and also will dramatically increase our understanding of their evolution in space, their relationship to carbon-dust ejecting objects, and the excitation conditions in each unique environment. ISO is well suited to measure spectra in regions of low brightness, precisely where important emission spectral changes are expected to occur. Emission spectroscopy of the IR cirrus will determine if the emitters are related to the PAHs in other galactic objects and their intercloud variations. Finally far-IR spectroscopy of PAH emitting objects by ISO may permit the first identification of specific interstellar PAHs.

INTRODUCTION

Section 3.5 of the 1979 ISO (Infrared Space Observatory) assessment study begins with the statement, "Very little is known about interstellar dust with any certainty. Formation and destruction mechanisms are largely the subject of speculation, and size, shape, and composition are guessed at as well.

And yet the dust is of major astrophysical importance, not only as an interstellar constituent itself, but because of the central role it plays in many other processes". This despite the fact that the dust constitutes only a small fraction of the interstellar matter. Important examples of these other processes in which dust plays a decisive role include interstellar extinction, cloud heating by photoelectron ejection, radiation conversion from higher energy photons into infrared photons, interstellar molecule formation, and star and planet formation. The role the dust plays in *all* of these processes is determined by its precise composition which, until recently, has been largely guessed at. *Mid-Infrared spectroscopy of the dust is the only way to get this critical information.* This is because the fundamental vibrational frequencies of virtually all molecules comprised of the most abundant cosmic elements H, O, C, and N fall in the mid-IR (Fig. 1). Many of these vibrations are IR active, producing a characteristic absorption or emission spectrum for each species (Allamandola 1984).

During the past decade, ground-, air- and space-based infrared spectroscopic observations have revolutionized our understanding of interstellar dust and the roles it plays in different environments. This progress has been severely hindered however by the infrared "blind spots" produced by strong telluric absorptions. The mid-infrared spans the range from about 4000 to 500 cm^{-1} (2.5 - $20\text{ }\mu\text{m}$). As also shown in figure 1, of these 3500 cm^{-1} , about 670 have been inaccessible to astronomers due to strong atmospheric absorptions and about 750 cm^{-1} require an airborne platform, making access very limited. Hence, ISO will provide high quality spectra in the 19% of the celestial mid-infrared which has *never* been studied and dramatically increase the number of spectra in the 21% with limited access. Furthermore, broad coverage of about 200 cm^{-1} of the far-infrared will be available for the first time. Though generally not as powerful a diagnostic of composition as the mid-IR, the far-IR can provide very important complementary information concerning the physical nature of grains.

Thus ISO has the potential to nearly double our knowledge of the IR spectroscopic properties of interstellar dust and PAHs. In order to fully exploit ISO requires that laboratory data be available with which one can analyze the spectra ISO measures. To maximize the scientific return from this limited lifetime mission it is particularly important to have as much laboratory data available as possible prior to launch in order to plan an intelligent follow-up program before the cryogen runs out. This dictates that laboratory studies focus on the spectral properties of astrophysically relevant materials with important bands in the new regions and regions of limited access. As with all pioneering spectroscopic studies unexpected features will be found. Their uniqueness can only be recognized if archives of the appropriate laboratory data are available.

This paper is outlined as follows. In the next section, the new information anticipated from absorption studies of ices in dense clouds is presented, followed by a similar discussion focused on the more refractory dust in the diffuse medium. Then emission spectroscopy is discussed, with emphasis on interstellar PAHs and related species. Table 1 summarizes all of this.

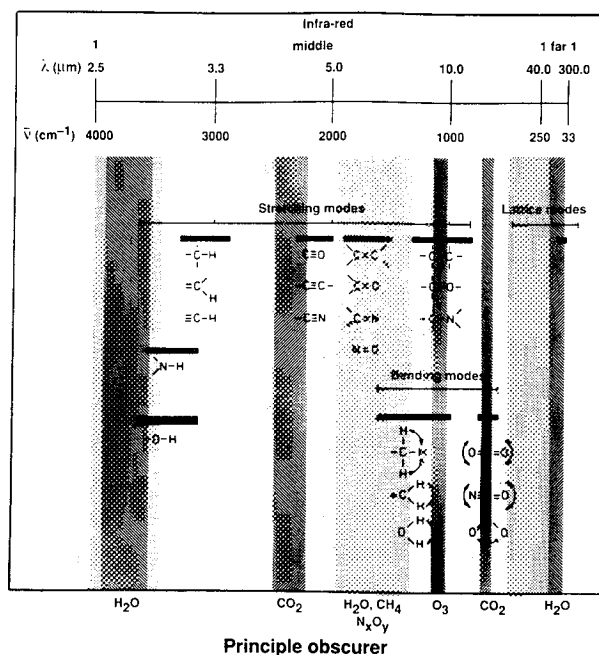


Fig. 1 Characteristic frequency ranges of chemical groups comprised of the most cosmically abundant elements H, O, C, and N (from Allamandola, 1984). The superposed bands show the regions opaque or obscured by the atmosphere. The lighter bands signify spectral regions of limited accessibility, requiring an airborne platform. The darker bands are inaccessible, requiring a spaceborne observatory such as ISO or SIRTf. The principle atmospheric species responsible are listed below each band.

ABSORPTION SPECTROSCOPY

Due to space limitations, a general discussion of how one can interpret astronomical infrared absorption spectra to derive composition, abundances, and chemical processes as given in Allamandola (1984) is not repeated here. Rather, emphasis is placed on new bands and spectra, assuming familiarity with the concepts presented earlier. Cross references to recent articles will be given to serve as doorways into the literature. For recent reviews of absorption spectroscopy of the dense and diffuse interstellar medium (ISM) see the respective chapters by Sandford (1993) and Pendleton (1993) in this book.

Dust in the Dense Medium

Absorption studies of protostars in dense molecular clouds probe the composition of dust and ices in the cloud itself and, in certain cases, of the protostellar-circumstellar environment (shell plus disk). ISO has the potential to determine the following important, but unknown, properties of ices in these objects:

- The deuterium-to-hydrogen (D/H) ratio
- The importance of CO_2 in ices and the amount of cosmic C in this molecule
- The importance of O_3 in ices and the amount of cosmic O in this molecule
- The importance of nitriles ($-C\equiv N$) and iso-nitriles ($C\equiv N-$) in ices and the amount of cosmic N in these species
- The relative amounts of isolated H_2O versus H_2O trapped in water ice lattices

Since it is not possible to discuss each potential new species and explore its importance in detail in the space available, the principal issues will be highlighted and references will be given when appropriate.

It has long been recognized that the distribution of deuterium (D) throughout the galaxy and the D/H ratio of the ISM are important in many areas of astrophysics. ISO has the potential to provide some of this information which cannot be obtained in any other way. Deuterium enrichments are known for some meteoritic components and gas-phase interstellar molecules. While these are considered very important indicators of interstellar processes and of processes influencing Solar System materials, the true extent of interstellar deuterium fractionation, and whether or not the derived D/H ratios suffer from selection effects associated with the specific molecules probed, is not known. Infrared spectroscopy of grains, on the other hand, has the potential to give the total, solid-state D/H ratio. This is because the stretching vibrations involving D and the most cosmically abundant elements fall in a narrow region of the infrared (Fig. 2). This may make it possible to determine the *entire* dust and ice D inventory in a single spectroscopic measurement between 2600 and 2000 cm^{-1} (3.9-5.0 μm). This measurement has the potential to provide CD/CH and OD/OH ratios as well. The bending and deformation modes also fall in a narrow range (Fig. 2), however these are likely to be overpowered by other interstellar bands. Although D is low in abundance with respect to hydrogen, two effects increase the likelihood of its detection: hydrogen-bonded OD stretches are significantly enhanced, and the bands all fall in a narrow range. Since interstellar ices are expected to contain a large fraction of the available deuterium (Tielens, 1983; Brown and Millar, 1989; Tielens, 1992), these measurements have the potential to resolve many uncertainties associated with the disposition of interstellar D and the role of grains in interstellar chemistry.

Theory and laboratory experiments indicate that carbon dioxide (CO_2) should be a common and very important component of interstellar ices (Tielens and Hagen, 1982; d'Hendecourt, Allamandola, and Greenberg, 1985; Allamandola, Sandford, and Valero, 1988). Naturally, the characteristic absorption bands of frozen CO_2 are obscured by telluric CO_2 . An extensive laboratory study of CO_2 frozen in a number of astrophysical ice analogs has shown that the CO_2 bands near 2340 and 670 cm^{-1} (4.27 and 15 μm) are not only diagnostic of this molecule, they can also provide important insight into the physical nature of the ice (crystalline, amorphous), the nature of the other constituents

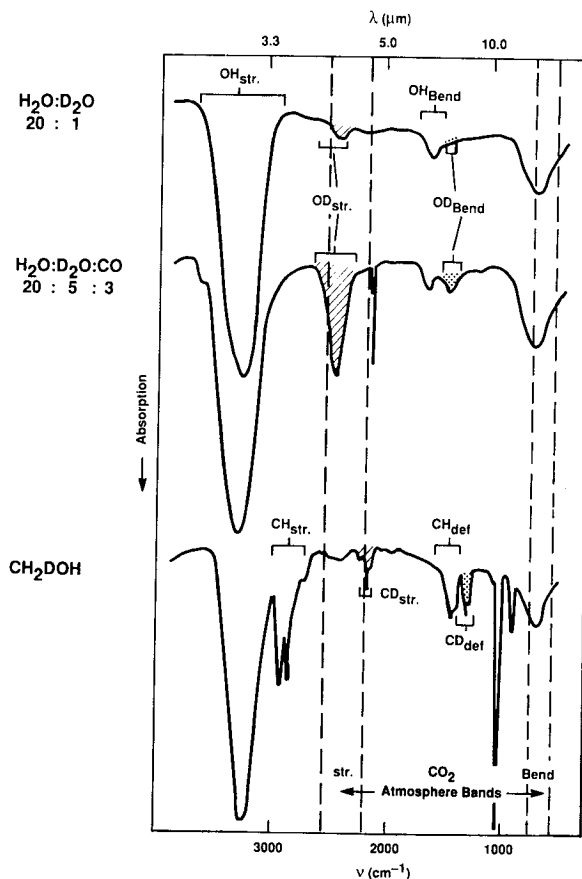


Fig. 2 Absorption spectra of deuterated ices at 10K. The shaded absorption bands are due to O-D and C-D fundamental stretching (str), bending (bend), and deformation (def) vibrations. The vertical bands show the regions obscured by atmospheric CO_2 , illustrating that space-borne instruments are required to search for the O-D and C-D stretching vibrations in ice and dust. N-D stretching vibrations fall here as well.

present (polar, nonpolar), as well as the ice's thermal history (Sandford and Allamandola, 1990). Furthermore, moderate resolution spectroscopy in the regions of these bands by ISO can probe the column densities of both frozen and gaseous CO_2 along the same lines-of-sight as discussed for CO in Allamandola (1984). d'Hendecourt and Jourdain de Muizon (1990) have reported the 667 cm^{-1} ($15\text{ }\mu\text{m}$) CO_2 band in IRAS-LRS spectra of a few clouds.

Ozone (O_3) is another likely ice component whose detection and study is obscured by its terrestrial counterpart. It is predicted to be an important oxygen reservoir in many interstellar chemistry models (Tielens and Hagen, 1982; d'Hendecourt, Allamandola, and Greenberg, 1985). Although its spectroscopic properties in astrophysical ices have not been reported it is well studied, having a strong band near 1035 cm^{-1} in a krypton matrix at 10 K (Brewer and Wang 1972). Unpublished results from the Ames laboratories indicate some

similarities with the solid state spectral effects found for CO_2 . Thus, studies of solid O_3 will provide insight into O-rich environments and, along with the CO_2 measurements, will give a good picture of the disposition of oxygen in dense clouds.

Nitriles ($-C\equiv N$) and isonitriles ($-N\equiv C$) are important chemical groups from a biological perspective. The fundamental vibration of the majority of these also absorb in the 2340 cm^{-1} region which is obscured by atmospheric CO_2 . Recently, a weak band near 4500 cm^{-1} ($2.22\text{ }\mu\text{m}$) was shown to be common to many Solar System bodies and has been assigned to the overtone of this vibration (Cruikshank et al. 1991). It is important to search for this fundamental in clouds as it affords a direct measure of the amount of nitrogen present. N_2 , a homonuclear diatomic, is IR inactive and NH_3 has not been unambiguously detected.

Water (H_2O) ice is well known from the deep 3250 cm^{-1} ($3.08\text{ }\mu\text{m}$) band. Less appreciated are important OH stretching vibrations in the $3700\text{--}3600\text{ cm}^{-1}$ ($2.7\text{--}2.8\text{ }\mu\text{m}$) range which arise from H_2O molecules which are not completely hydrogen-bonded to other molecules in the ice (Allamandola, 1984). Searching for these bands is important. Their presence or absence can tell much about the condensation conditions and thermal history of grains in a particular region. The abundance of H_2O in ices is uncertain and there may well be significant amounts of H_2O present in this form. Examples of this feature in many binary ice mixtures are given in Hagen, Tielens, and Greenberg (1983).

Dust in the Diffuse Medium

Compared to our knowledge of dust in dense clouds, our knowledge of dust composition in the diffuse medium is in its infancy. This is because the amount of spectral information available is limited both in spectral range coverage, and in objects studied due to the inherent weakness of the features toward sources associated with low values of A_v . Most conclusions are based on the OH/NH/CH stretch region of the galactic center sources. Recently several other sources have also been studied, but the data is generally not of the same quality as that of the galactic center sources. Thus, it is particularly important that enough ISO time be devoted to obtain high quality, good signal-to-noise spectra of several representative lines-of-sight through the diffuse ISM. The current situation in this field is reviewed by Pendleton (1993) elsewhere in this volume.

Critical questions concerning dust in the diffuse medium which ISO can address include the determination of its spectral characteristics in *all* of the obscured bands along several lines-of-sight. As with the dense medium, these measurements may reveal the D/H ratio and probe the importance of biogenic nitriles. Of particular interest is the region from $2000\text{--}1200\text{ cm}^{-1}$ ($5\text{--}8\text{ }\mu\text{m}$) as this carries information regarding the precise nature of the organic component. Although accessible from an airborne platform, the sensitivity provided by ISO and future spaceborne instruments is required to obtain spectra of sufficient quality along several lines-of-sight. These spectra are essential if one is to make valid comparisons with the spectral properties of: interplanetary dust particles

(IDPs), the organic residues produced in laboratory simulation experiments, and extracts from meteorites. It is only through such comparisons that one can learn the true nature of dust in the diffuse interstellar medium, and the extent of the connection (if any) between the diffuse ISM and Solar System materials.

EMISSION SPECTROSCOPY

Spectroscopic studies of IR emitting objects by ISO in the obscured regions are needed to provide critical information which can complement and complete the extensive work carried out from ground based and airborne observatories. Emphasis should also be placed on exploiting ISO's unique capabilities and high sensitivity by studying faint sources and transition zones where current instrumentation fails. It is at these locations that emission spectra reveal the effects of radiation field variations and the structure and chemical evolution of the emitting species. These studies, emphasizing PAH emission objects, are of considerable importance because fully 20-30% of all galactic IR radiation is emitted by PAHs and PAH related macromolecules (VSGs ?) and micrograins; PAHs are more abundant than all other known interstellar polyatomic molecules combined; molecular PAHs contain 1-5% of the cosmic carbon; and macromolecular PAHs and micrograins about 20-30% (Allamandola, Tielens, and Barker, 1989; Puget and Leger, 1989). Following the spectral evolution of the emission from regions of low UV flux, which have not been well studied, to regions of higher excitation (eg. Geballe et al. 1989) will provide tell-tale signatures of carbon's cosmic evolution and may provide insight into the relationship between free molecular PAHs and amorphous carbon grains.

ISO has the potential to determine the following fundamental, but unknown, properties of PAHs and amorphous carbon grains in many objects:

- The D/H ratio in PAHs and D distribution in IR emitting objects
- The spatial distribution of molecular PAHs versus the distribution of PAH clusters and amorphous carbon particles in extended objects
- The identity of specific PAHs

Small PAHs are expected to be heavily D enriched (Allamandola, Tielens, and Barker, 1989). These are the same small PAHs which dominate the emission at the highest infrared frequencies. In a fully deuterated PAH, the CD stretch is the highest frequency fundamental. As illustrated in Fig.3, this aromatic CD stretch shifts to a position obscured by telluric CO_2 . Thus studying this region of the brightest PAH emission objects known has the potential to provide information related to the D/H ratio in small PAHs and the emission zones.

Tracking the spatial behavior of the narrow CC stretching features attributed to free, molecular, ionized PAHs such as the 1610 cm^{-1} ($6.2\text{ }\mu\text{m}$) band

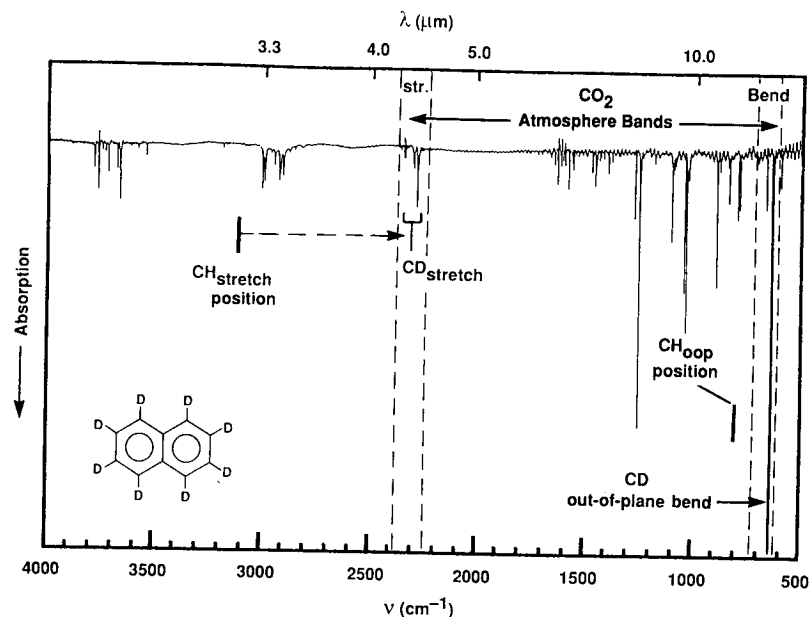


Fig. 3 Absorption spectrum of the deuterated PAH, naphthalene (C_{10}D_8), isolated in an argon matrix at 10K. The aromatic CD stretch falls near the center of the atmospheric CO_2 stretching band and the aromatic CD out-of-plane (oop) bend falls at the low frequency end of the atmospheric CO_2 bending mode. The bold vertical bars indicate the position of the aromatic CH stretching and bending vibrations.

versus that of the pedestal under this and the "1300" cm^{-1} ("7.7" μm) bands attributed to clusters, macromolecules, and grains and comparing these spatial behaviors with similar studies of the CH stretching and bending bands (3100-2700 and 900-500 cm^{-1} , 3.2-3.7 and 11-20 μm) is equivalent to following the form and evolution of carbon. This can be investigated as a function of excitation in C- rich objects at different stages of evolution by comparing spectra from red-giants to spectra of proto-planetary and planetary nebulae. It will also be of extreme interest to compare the spectra from H-II regions with the complete spectra of reflection nebulae and of the IR cirrus. Very little is known about the details of the emission spectra from low brightness objects such as reflection nebulae and the IR cirrus clouds. The spectrum of the IR cirrus is presumed to be PAH-like. It will be very interesting to find out if this is indeed the case and, if so, how the cirrus spectra compare in detail. Band positions, relative intensities, and profiles are indicators of structure and size, thus affording a powerful probe of conditions in the high latitude cirrus clouds.

Finally, since PAH plane-bending modes are characteristic of specific PAHs, the LWS spectrometer on ISO provides a very real opportunity to identify specific interstellar PAHs.

OPAQUE REGION		TARGET BAND CARRIERS	
Frequency, cm ⁻¹ (μ m)	Obscurer	Absorption	Emission
4000 -3650 (2.5 - 2.75)	[H ₂ O]	Free H ₂ O	?
2440-2250 (4.1 - 4.4)	[CO ₂]	CD, OD, CO ₂ , C \equiv Nstretches	PAD:CD stretch
1960-1100 (*5.1 - 9)	H ₂ O, CH ₄ , N _x O _y ,...	Organics >C=O	PAH:C-Cstretch (most intense)
1050-1000 (9.5 - 10)	[O ₃]	O ₃	?
750-600 (13 - 17)	[H ₂ O, CO ₂]	CD, OD, O ₃ , CO ₂ , \equiv C-H bends	PAD:CD bend
<200 (>50)	[H ₂ O]	Ice phonons	PAH plane bends

* Limited access - requires airborne platform.

Table 1: Frequency regions and target bands related to interstellar dust which will be pioneered by ISO.

CONCLUSION

Summing up, as indicated by Table I, the absorption spectra ISO obtains will shed light on D/H ratios, composition, abundances, and chemical processing of ices and dust in dense molecular clouds, the diffuse interstellar medium and in cold disks. In many cases gas phase column densities of the same molecules can be measured along the same lines-of-sight. Emission spectra will shed light on PAH D/H ratios and compositional variations as a function of object type along the H-R diagram and the relationship of PAHs (if any) to the IR cirrus.

To interpret the absorption spectra, infrared spectroscopic studies should be carried out on realistic astrophysical ice analogs containing the species and subgroups listed in the third column of the table. For the emission bands, studies are needed on isolated, neutral and ionized polycyclic aromatic hydrocarbons which are hydrogenated (PAHs) and deuterated (PADs).

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